

Existence and transitions properties of three–deuteron muonic molecule ($3d\,2e^-\,\mu^-$)

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Abstract

We calculated the energy and the size of the three-deuteron muonic molecule ($3d\,2e^-\,\mu^-$) = $D_3\mu$. It turns out that this system possesses two equilibrium positions, one at distances typical for muonic molecules and a second one at the usual molecular size. We show, moreover, that the fusion probability of the three deuterons is considerably enhanced due to the existence of a ${}^6\text{Li}^*$ threshold resonance. Our estimates indicate that this probability is considerably higher than the decay rate of the competing Auger transition.

I. INTRODUCTION

The physics of two-atomic muonic molecules, as $pp\mu$, $dd\mu$ or $dt\mu$, has a long and intense history since the prediction of such molecules in the forties and their discovery in the fifties [1]. Unfortunately, attempts to produce energy for practical use by muon-catalyzed fusion in the $dt\mu$ case, the most promising candidate, were up till now unsuccessful. However, the corresponding investigations revealed some peculiar aspects of the molecular and nuclear physics of such systems. Muonic molecules, e.g., offer the possibility of measuring the strong interaction between charged nuclei at very low energies ($E \sim \text{eV}$) which, without the Coulomb shielding by μ^- , is not accessible to experiment under normal laboratory conditions.

An important aspect of these systems, pointed out in [2–5], concerns the formation of threshold resonances of the nuclei involved, which leads to a considerable enhancement of their fusion probability. Such resonances occur in a number of systems, as $dt\mu$, $t\ ^3\text{He}\mu$ or $d\ ^6\text{Li}\mu$. In the $dt\mu$ case [1], for example, the near-threshold state $^5\text{He}(3/2^+)$ increases the cross section for the nuclear transition

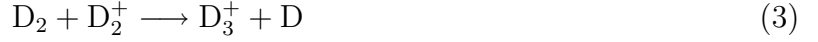
$$dt\mu \longrightarrow ^5\text{He}(3/2^+)\mu \longrightarrow ^4\text{He} + \mu + n \quad (1)$$

by four orders of magnitude as compared to reactions where no threshold resonances occur.

In the present work we investigate an analogous three-atomic situation, namely, the system ($3d2e^- \mu^- = \text{D}_3\mu$) in which one of the electrons in the deuterium molecule ($3d3e^- = \text{D}_3$) is replaced by a muon. Fig. 1. shows that three deuterons can form two $^6\text{Li}^*$ resonances at energies very close to the $3d$ threshold energy, $E_{th}^{3d} = 25.32 \text{ MeV}$, i.e., to the energy just needed to disintegrate ^6Li into three deuterons. This indicates that in $\text{D}_3\mu$ three-body fusion can take place enhanced by the formation of the $(J^\pi, T) = (3^-, 0)$ resonance,

$$3d\mu \longrightarrow ^6\text{Li}^*(3^-, 0) + \mu. \quad (2)$$

It is interesting to note that the D_3 molecule and its D_3^+ ion are stable and have quite peculiar spectra [7]. The D_3^+ ion can be produced in the collision



with a high formation probability of the order of $\lambda \sim 10^9 \text{ cm}^{-3} \text{ sec}^{-1}$. Thus, it can be easily produced under laboratory conditions [8]. We also mention that the hydrogen analog H_3^+ of the deuterium ion D_3^+ , discovered already at the beginning of this century by J.J. Thompson [9], plays an important role in the atmosphere of Jupiter and, in general, in astrochemistry where it protonates the otherwise chemically inactive CO molecule [10],



It is, therefore, expected that a sufficient number of $D_3\mu$ molecules can be produced via the D_3^+ production and a subsequent μ^- capture, so that there is enough material for the 3d fusion process.

In Sect. II we calculate the energy and the size of the $D_3\mu$ molecule using a Born-Oppenheimer-type ansatz for the wave function. An estimation of the nuclear transition rate and, in particular, of the enhancement factor due to the intermediate ${}^6\text{Li}^*$ resonance formation is obtained in Sect. III. In order to compare this rate with the magnitude of the conventional atomic decay of this molecule, we estimate in Sect. IV the corresponding Auger transition probability. Our conclusions are drawn in Sect. V. Finally some technical details concerning the Auger transition are presented in the Appendix.

II. ENERGY AND SIZE OF $D_3\mu$

We assume the motion of the heavy particles, the deuterons, to be of adiabatic character and therefore their kinetic energy in the total Hamiltonian

$$\hat{H} = -\frac{1}{2m_e}(\Delta_{\boldsymbol{\rho}_1} + \Delta_{\boldsymbol{\rho}_2}) - \frac{1}{2m_\mu}\Delta_{\mathbf{r}} + \frac{1}{|\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2|} + \frac{1}{|\mathbf{r} - \boldsymbol{\rho}_1|} + \frac{1}{|\mathbf{r} - \boldsymbol{\rho}_2|}$$

$$-\sum_{i=1}^3 \frac{1}{|\mathbf{r}_i - \boldsymbol{\rho}_1|} - \sum_{i=1}^3 \frac{1}{|\mathbf{r}_i - \boldsymbol{\rho}_2|} - \sum_{i=1}^3 \frac{1}{|\mathbf{r}_i - \mathbf{r}|} + \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \quad (5)$$

can be omitted. Here $\boldsymbol{\rho}_1$, $\boldsymbol{\rho}_2$, and \mathbf{r} are the coordinates of the electrons and the muon in the center-of-mass (CM) system (see Fig. 2) of the three deuterons. The \mathbf{r}_i denote the coordinates of the deuterons.

For the ground state of the $D_3\mu$ molecule we use the ansatz

$$\Psi = \psi(R, \chi, \theta) \left(e^{-\alpha/2(\mathbf{r} - \nu\mathbf{r}_1)^2} + e^{-\alpha/2(\mathbf{r} - \nu\mathbf{r}_2)^2} + e^{-\alpha/2(\mathbf{r} - \nu\mathbf{r}_3)^2} \right) e^{-\kappa/2\rho_1^2 - \kappa/2\rho_2^2} \quad (6)$$

where in the three-deuteron wave function $\psi(R, \chi, \theta)$ the following hyperspherical variables were chosen instead of the position vectors \mathbf{r}_i ,

$$R^2 = x^2 + y^2, \quad \tan \chi = \frac{y}{x}, \quad \cos \theta = \frac{\mathbf{x} \cdot \mathbf{y}}{xy}, \quad \Omega \equiv (\chi, \theta) \quad (7)$$

where

$$\mathbf{x} = \sqrt{\frac{1}{2}}(\mathbf{r}_1 - \mathbf{r}_2), \quad \mathbf{y} = \sqrt{\frac{2}{3}} \left(\mathbf{r}_3 - \frac{(\mathbf{r}_1 + \mathbf{r}_2)}{2} \right). \quad (8)$$

Employing the ansatz (6) in a minimization procedure in which the parameters α , ν and κ at fixed values of \mathbf{r}_i are varied, we obtain the corresponding energy surface $U(R, \chi, \theta)$, the effective interaction of the deuterons. Due to its variational origin, this potential will provide an upper bound to the exact eigenvalue of \hat{H} at any pair of angles χ and θ . As can be seen in Figs. 3 and 4, the minimum of this function at different values of R is reached for $\chi_0 = \pi/4$ and $\theta_0 = \pi/2$, i.e., for an equilateral position of the three deuterons. Therefore, the ground state for the three-deuterons should appear essentially in this symmetric configuration and thus the potential $U_0(R) = U(R, \chi_0, \theta_0)$ can be employed to calculate $\psi(R, \chi, \theta)$. This is supported by the fact that, due to the almost classical motion of the heavy particles, the ground state energy will be close to the minimum of the potential surface shown in Fig. 3

and 4. The dependence on α , ν and κ on R is shown in Fig. 5 while in Fig. 6 we plot $U_0(R)$ versus the hyperradius R . As can be seen, $U_0(R)$ has two minima, the first one at “muonic” distances and the second one at atomic distances. The later minimum, obviously, corresponds to the case where one of the deuterons in a D_2 molecule, is replaced by the $dd\mu$ bound system.

The eigenvalue equation for the 3d states reads

$$\left(-\frac{1}{2m_d} \frac{1}{R^5} \frac{\partial}{\partial R} R^5 \frac{\partial}{\partial R} + \frac{1}{2m_d} \frac{\Lambda^2}{R^2} + U_0(R) \right) \psi(R, \Omega) = \mathcal{E}_3 \psi(R, \Omega), \quad (9)$$

with

$$\Lambda^2 = \frac{4}{\sin^2 \chi} \left(\frac{\partial}{\partial \chi} \sin^2 \chi \frac{\partial}{\partial \chi} + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} \right) \quad (10)$$

Due to the Ω -independence of $U_0(R)$, the solutions of (9) can be written as

$$\psi(r, \Omega) = X(R) \mathcal{Y}_{\mathcal{L}}(\Omega), \quad (11)$$

where the hyperspherical harmonics $\mathcal{Y}_{\mathcal{L}}(\Omega)$ satisfy the eigenvalue equation

$$\Lambda^2 \mathcal{Y}_{\mathcal{L}} = \mathcal{L}(\mathcal{L} + 1) \mathcal{Y}_{\mathcal{L}} \quad (12)$$

of the grand angular momentum operator Λ . The quantum number $\mathcal{L} = n + l_1 + l_2 + 3/2$ is composed of the angular momenta l_1 and l_2 corresponding to the Jacobi coordinates \mathbf{x} and \mathbf{y} , while n denotes the degree of the relevant Jacobi polynomial.

In a wide range of R ($0.1 \leq R \leq R_0$) and for the quantum number $\mathcal{L} = 5/2$ (relevant in our context) we have

$$\frac{\mathcal{L}(\mathcal{L} + 1)}{2m_d R^2} \ll |U_0(R)|. \quad (13)$$

Equation (9) thus reduces to

$$\left(-\frac{1}{2m_d} \frac{1}{R^5} \frac{\partial}{\partial R} R^5 \frac{\partial}{\partial R} + U_0(R) \right) X(R) = \mathcal{E}_3 X(R). \quad (14)$$

Having in mind the extremely large width of the barrier between the two minima of the potential $U_0(R)$ one can consider the states bound by the short-range minimum as physically stable with respect to a decay into the second-minimum states. In this area the potential can be approximated fairly well by

$$U_0(R) = a + b(R - \bar{R})^2. \quad (15)$$

The constants a and b were found to be (we use the units $e = \hbar = m_\mu = 1$)

$$a = 0.31, \quad b = 0.01, \quad \bar{R} = 4.45. \quad (16)$$

Equation (14) can then be easily solved with the results for the energy and the size of $D_3\mu$ being

$$\mathcal{E}_3 = -1.74 \text{ keV}, \quad R_0 = 11.0 \cdot 10^{-11} \text{ cm}. \quad (17)$$

Both values are of the same order of magnitude as the ones of the corresponding two-atomic muonic molecule ($\mathcal{E}_2 \sim -2.7 \div -2.8 \text{ keV}$, $R_0 \sim 5 \cdot 10^{-11} \text{ cm}$) [1].

Apart from effects due to the ${}^6\text{Li}$ resonance formation (see forth section III) comparable nuclear transition rates should be expected in both systems.

III. NUCLEAR TRANSITIONS

According to Fig. 1 there are two ${}^6\text{Li}^*$ resonances with energies close to the $3d$ threshold. The lowest one for the $(J^\pi, I) = (4^-, 1)$ quantum numbers is given by $E + i\Gamma = (25 + i4) \text{ MeV}$ and the higher one for $(J^\pi, T) = (3^-, 0)$ [12] which has a broad width $E = 26.6 \text{ MeV}$. Since the isospin of the deuteron is zero, the $3d$ state can undergo a fusion reaction only via the latter resonance, and hence the $D_3\mu$ molecule has to be in a $J^\pi = 3^-$ state.

Following the procedure suggested in [11], the probability of the nuclear fusion is obtained from the overlap integral \mathcal{M} between the molecular and resonance wave functions, i.e., from

$$w = \mathcal{E}_3 |\mathcal{M}|^2. \quad (18)$$

In contrast to the calculations of the energy and the size of the $D_3\mu$ molecule, where simple approximations such as (15) were sufficient, the calculations of the overlap integral is much more delicate. This is due to the fact that the wave function of the three outgoing charged particles in the near-threshold region we are interested in, is highly oscillatory. Thus, in order to avoid direct numerical integrations we choose wave functions that describe the crucial input for the $D_3\mu$ molecule and the ${}^6\text{Li}$ resonance, and allow us to perform the integrations analytically.

For this purpose we approximate the potential $U_0(R)$ at short distances by an analytic function. This is easily achieved by using the effective Coulomb potential Z_{eff}/R . The effective charge Z_{eff} can be found by fitting the eigenpotential $U_0(R)$ at small distances the result being $Z_{eff} = 2.8$. In this region the wave function is, therefore, given by the regular Coulomb solution $F_{\mathcal{L}}(R)$.

At large distances the wave function decrease exponentially and therefore we may use a phenomenological anzatz of the form

$$\psi_{mol} = \frac{N_m}{R^{\frac{5}{2}}} F_{\mathcal{L}}(\eta, kR) e^{-kR} Y^{J,M}(\hat{x}, \hat{y}) u_{\mathcal{L}}(R), \quad (19)$$

which describes both the size of the molecule and the Coulomb repulsion of the three deuterons at small distances. N_m is the normalization constant, $\eta = Z_{eff}m_d/k$ is the Sommerfeld parameter, and $k = \sqrt{2m_d|\mathcal{E}_3|}$. $Y^{J,M}(\hat{x}, \hat{y})$ are the bispherical harmonics corresponding to the total angular momentum J . Since we assume the molecule to be in the ground state with negative parity, we have $n = 0$ and for the sum of the relative angular momenta $\ell_1 + \ell_2 = 1$. In other words we have $\mathcal{L} = 5/2$.

Due to the repulsion of the deuterons at small distances, the wave function (19) is exponentially small in this region. This means, the main contribution to the overlap integral comes from distances R much larger than the nuclear size r_0 and thus we may use the asymptotic

form of the ${}^6\text{Li}^*$ resonance state which is taken to be the asymptotic wave function of three charged particles in the continuum

$$\psi_{res}(R, \Omega) = \frac{N_{res}}{R^{5/2}} f^J(R, \omega) Y^{J,M}(\hat{x}, \hat{y}), \quad (20)$$

where

$$f^J(R, \omega) = \int \exp[iqR + \frac{iv(\Omega)}{q} \ln(qR)] Y^{J,M}(\hat{x}, \hat{y}) d\hat{x}d\hat{y}$$

The factor N_{res} represents the normalization in the nuclear volume and the angles are denoted by $\Omega \equiv (\omega, \hat{x}, \hat{y})$; $v(\Omega)$ represents the angular part of the total Coulomb potential of the three-body systems written in terms of hyperspherical variables while $q = \sqrt{2m_d|E - E_{th}|}$ with E being the energy of the outgoing particle and E_{th} the threshold energy.

After some tedious calculations, with $\eta(\Omega) \equiv v(\Omega)m_d/q \approx \eta \gg 1$, and $u_{\mathcal{L}}(R) = 1$, we found that the overlap integral,

$$\mathcal{M} = \int \psi_{res}(R, \Omega) \psi_{mol}(R, \Omega) R^5 dR d\Omega, \quad (21)$$

has the behavior

$$\mathcal{M} \sim e^{\pi\eta(\Omega_1)(\frac{iS(t_-)}{\pi} - \frac{1}{2})}, \quad (22)$$

with

$$\gamma = \frac{q}{k}, \quad \sigma = \frac{v(\Omega_1)}{Z_{eff}} = 1.06,$$

$$S(t) = [-\ln(t) + \ln(1-t)] \frac{\gamma}{\sigma} + \ln(1 - i(\gamma - 1) - 2it),$$

and

$$t_- = \frac{\sigma - \gamma}{2\sigma} - \frac{1}{2\sigma} \sqrt{\gamma^2 + \sigma^2 - 2\gamma\sigma[\gamma + i]}.$$

Ω_1 is obtained from the condition

$$\nabla v(\Omega) = 0$$

and turns out to be the same as $\Omega_0 \equiv (\chi_0, \theta_0)$ introduced above. It should be noted that any other reasonable choice of $u_{\mathcal{L}}(R)$ is not expected to lead to a significant modification of \mathcal{M} .

From (22) it follows that an enhancement of the transition rate is achieved if

$$\text{Im } S(t_-) < 0, \quad \frac{|\text{Im } S(t_-)|}{\pi} > \frac{1}{2}. \quad (23)$$

In Table I we present the $\text{Im } S(t_-)/\pi$ for certain values of the parameters γ . Evidently the condition (23) is satisfied. In other words, the usual decreasing Coulomb barrier is replaced by a factor which grows with increasing η . Since in the present case (near threshold reactions) $\eta \gg 1$, a considerably enhanced transition of the three deuterons into the ${}^6\text{Li}^*(3^-, 0)$ resonance is to be expected. The corresponding transition probabilities are given in the last column of Table I. The above nuclear fusion process is accompanied by a radiative $E1$ transition into the ${}^6\text{Li}$ ground state yielding an energy of about 26 MeV .

IV. AUGER TRANSITION RATE

Since the binding energy of $\text{D}_3\mu$ is essentially higher than the one obtained for the $dd\mu$ -molecule [6], we have also as a possible decay process the Auger transition which for the $\text{D}_3\mu$ molecule is given by

$$\text{D}_{3\mu} \longrightarrow X + e^- . \quad (24)$$

Here X includes the $dd\mu$ molecule, the deuteron d , and a second (bound) electron e^- . To specify the wave function of the system X the following arguments can be used. In the Auger transition (24) most of the energy released is taken by the outgoing electron. This means that the relative velocity of the $dd\mu$ molecule and a nucleus d in the final state, is much smaller as compare to the velocities of electrons. Furthermore having in mind the small distances between all three deuterons in the initial state, one can consider the bound electron as moving in the Coulomb field of a “united” atom, formed by the $(dd\mu)^+$ ion and the nucleus d .

The transition rate for this mode of decay is, of course, quite essential and is of relevance to the competing nuclear transition. The corresponding transition probability is determined from the amplitude

$$\mathcal{M}_A = \langle \psi_f | V_C | \psi_i \rangle, \quad (25)$$

where V_C is the Coulomb interaction of the outgoing electron with the second electron and with the center of mass the complex $[dd\mu + d]$. The initial state ψ_i is the $D_3\mu$ wave function described Sec. II, Eq. (6). The final state ψ_f is chosen to be a product of the wave functions of the fragments, namely,

$$\psi_f = \psi_{rel} \psi_{at} \phi_{out} \psi_{dd\mu} \quad (26)$$

where ψ_{rel} is the Coulomb wave function for the relative motion of the $dd\mu$ molecule and the deuteron d , ψ_{at} is the atomic wave function of the bound electron in the field of the $dd\mu + d$ system, ϕ_{out} is the plane wave function of outgoing electron, and $\psi_{dd\mu}$ is the ground state wave function of the $dd\mu$ molecule which is assumed to be of the form

$$\psi_{dd\mu} = \sqrt{\frac{\zeta^3}{\pi a_\mu^3}} e^{-\zeta r_d/a_\mu} \psi_{dd\mu}^{LCAO} \quad (27)$$

where $\psi_{dd\mu}^{LCAO}$ designates the Linear Combination of Atomic Atomic Orbitals (LCAO) wave function,

$$\psi_{dd\mu}^{LCAO} = \frac{1}{\sqrt{2(1+F(r_d))}} \frac{1}{\sqrt{\pi a_\mu^3}} \left(e^{-|\mathbf{r}_d/2 - \mathbf{r}_\mu|/a_\mu} + e^{-|\mathbf{r}_d/2 + \mathbf{r}_\mu|/a_\mu} \right), \quad (28)$$

with

$$F(r_d) = \left(1 + \frac{r_d}{a_\mu} + \frac{1}{3} \left(\frac{r_d}{a_\mu} \right)^2 \right) e^{-r_d/a_\mu}.$$

a_μ is the Bohr radius for the $d\mu$ atom, r_d the distance between the deuterons, r_μ is the muon Jacobi coordinate in the $dd\mu$ system, and $\zeta = 0.023$ is a constant that characterizes the size of the $dd\mu$ molecule. Due to the comparatively large size of the $D_3\mu$ molecule, it is enough to use a $dd\mu$ wave function of the form (27) which provides the correct binding energy and has the correct behavior at large distances.

The width for the Auger transition (24) is defined by (see the Appendix)

$$\frac{\Gamma}{2} = \frac{\mu_D e^4}{\hbar^2 16 \pi^3} \int_0^1 dx \frac{|\mathcal{M}_A(x, \tilde{q}(x))|^2}{\tilde{q}(x)} \quad (29)$$

where

$$\begin{aligned} x &= \frac{k}{k_0}, & \tilde{q}(x) &= \sqrt{\frac{\mu_D(1-x^2)}{\mu_e}}, \\ k_0 &= \sqrt{\frac{-2\mu\mathcal{E}_3}{\hbar^2}}, & \mu_D &= \frac{m_d(2\mu_d + m_\mu)}{3m_d + m_\mu}. \end{aligned}$$

Numerical integration of $|\mathcal{M}_A|^2$ over all final state momenta permitted by the energy-momentum conservation yields the decay rate

$$\lambda = \frac{\Gamma}{\hbar} \approx 10^{15} \text{sec}^{-1}. \quad (30)$$

V. CONCLUSIONS

Our calculations show that the effective potential energy for the three-deuterons in the $D_3\mu$ system possesses two equilibrium positions the first being at a distance characteristic for muonic molecules while the second one is of the same order of magnitude as that of the usual electronic molecules. The position and value of the “atomic” minimum of the effective potential energy imply the following cluster structure of the $D_3\mu$ system at this distance

$$\Psi_{D_3\mu} \approx \Psi_D + \alpha \Psi_{(dd\mu)e}, \quad (31)$$

where Ψ_D is the wave function of the hydrogen atom and $\Psi_{(dd\mu)e}$ is a hydrogen-like wave function with the $dd\mu^+$ ion in the center of such “atom”. One should bear in mind that such a clustering ensures the lowest possible energy of the system $D_3\mu$. Indeed, as can be seen in Fig. 4, this is just the case. It is obvious, that such a state of the $D_3\mu$ system is stable as far as electromagnetic transitions are concerned, but it is not stable with respect to nuclear fusion in the $dd\mu$ subclusters.

Let’s now discuss in brief the possibility of observing the $D_3\mu$ system. One way is to search for the Auger electrons with kinetic energy around 1 keV. A second possibility is, of course, more exotic and consists in observing the products of the triple fusion and the formation of the highly excited state $(3^-, 0)$ at 26.6 MeV of the 6Li nucleus.

The enhancement factor of the nuclear transition in the $D_3\mu$ molecule, obtained above, should be considered as an indication of the possible strong influence of the near-threshold nuclear resonance on the molecular system.

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APPENDIX A: EVALUATION OF THE AUGER TRANSITION

For the width Γ the following definition has been used:

$$\frac{\Gamma}{2} = \int \pi \frac{\mathcal{M}_A}{2kq} \delta \left(E - \frac{\hbar^2 k^2}{2\mu_e} - \frac{\hbar^2 q^2}{2\mu_D} \right) \frac{\mathcal{M}_A^*}{2kq} \frac{d^3 k}{(2\pi)^3} \frac{d^3 q}{(2\pi)^3}. \quad (\text{A1})$$

The matrix elements for the Auger transition \mathcal{M}_A (25) are given by

$$\begin{aligned} \mathcal{M}_A = & \int d^3 r_D d^3 \rho d^3 r_d d^3 r_\mu d^3 r_e \Psi_{dd\mu}(r_d, r_\mu) \frac{F_0(\eta, qr_D)}{r_D} \frac{\sin(k\rho)}{\rho} \frac{2^{3/2}}{\sqrt{\pi a_e^3}} e^{-2r_e/a_e} \\ & N_{var} \left(-\frac{2}{\rho} + \frac{1}{|\boldsymbol{\rho} - \mathbf{r}_e|} \right) e^{-\frac{k}{2}\rho^2} e^{-\frac{k}{2}r_e^2} \left(\sum_{i=1}^3 e^{-\frac{\alpha}{2}(\mathbf{r}_\mu - \frac{1}{3}\mathbf{r}_D - \nu\mathbf{r}_i)^2} \right) X(R), \end{aligned} \quad (\text{A2})$$

where N_{var} is the normalization constant of the variational part of the wave function (6)

and r_D is the Jacobi coordinate of the third deuteron not belonging to the $dd\mu$ molecule.

After some analytical derivations, one remains with the following simplified form

$$\begin{aligned} \mathcal{M}_A(k, q) = & \frac{16}{\pi^{7/4}} \frac{2^{3/2}\sqrt{\zeta}}{a_e} \left(\frac{a_\mu}{a_e} \right)^{1/2} \int \frac{d^3 r_d d^3 r_D}{\sqrt{3 \left(1 + 2 \exp \left(-\frac{1}{4} \alpha \nu^2 R^2 \right) \right)}} \frac{\kappa^{3/2}}{\alpha^{3/4}} \frac{e^{-\zeta r_d}}{\sqrt{2(1 + F(r_d))}} \\ & \left(\sum_{i=1}^3 I_+^{(i)} + I_-^{(i)} \right) \frac{F_0(\eta, qr_D)}{r_D} \left(-\mathcal{J}(\kappa/8) \left(\frac{a_e}{a_\mu} \right) \frac{k}{4\kappa} \mathcal{K}(k^2/\kappa) + \mathcal{I} \left(\kappa/2, k \frac{a_e}{a_\mu} \right) \right) X(R) \end{aligned} \quad (\text{A3})$$

where

$$R^2 = \frac{1}{2}r_d^2 + \frac{2}{3}r_D^2, \quad I_\pm^{(i)} = \frac{4\pi}{\sqrt{\alpha}d_{i\pm}} e^{-\alpha \frac{d_{i\pm}^2}{2}} \mathcal{R} \left(\frac{1}{\sqrt{\alpha}}, \sqrt{\alpha d_{i\pm}^2} \right),$$

$$\mathcal{R}(\xi, \sigma) = -\frac{\sqrt{2\pi}}{4} \left[(\xi - \sigma) e^{-(\xi - \sigma)^2/2} \operatorname{erfc} \left(\frac{\xi - \sigma}{\sqrt{2}} \right) - (\xi + \sigma) e^{-(\xi + \sigma)^2/2} \operatorname{erfc} \left(\frac{\xi + \sigma}{\sqrt{2}} \right) \right],$$

$$\vec{d}_{i\pm} = \frac{1}{3}\vec{r}_D \pm \frac{1}{2}\vec{r}_d + \nu\vec{r}_i, \quad \mathcal{K}(x) = \sum_{n=1}^{\infty} \frac{(-x)^{n-1}}{(2n-1)!!}.$$

$$\mathcal{J}(\alpha) = -\frac{1}{4\alpha^2} + \sqrt{\frac{\pi}{\alpha^5}} \frac{1/2 + \alpha}{4} e^{\frac{1}{4\alpha}} \left(1 - \operatorname{erf} \left(\frac{1}{2\sqrt{\alpha}} \right) \right)$$

$$\mathcal{I}(\alpha, \delta) = \int_0^\infty dx x \sin(\delta x) e^{-\alpha x^2} \left(\frac{1}{x} J_1(x, \alpha) + J_2(x, \alpha) \right)$$

$$J_1(x, \alpha) = e^{1/\alpha} \left\{ \frac{1}{2\alpha^{3/2}} \left[\gamma(3/2, \alpha(x + 1/\alpha)^2) - \gamma(3/2, 1/\alpha) \right] - \frac{1}{\alpha^2} \left[e^{-1/\alpha} - e^{-\alpha(x + 1/\alpha)^2} \right] - \frac{1}{2\alpha^2} \sqrt{\frac{\pi}{\alpha}} \left[1 - \operatorname{erf} \left(\sqrt{\alpha}(x + 1/\alpha) \right) \right] \right\} ,$$

and

$$J_2(x, \alpha) = e^{1/\alpha} \frac{1}{2\alpha} \left(e^{-\alpha(x + 1/\alpha)^2} - \sqrt{\frac{\pi}{\alpha}} \left[1 - \operatorname{erf} \left(\sqrt{\alpha}(x + 1/\alpha) \right) \right] \right) .$$

We note here that in (A3) the following dimensionless variables $\alpha a_\mu^2 \rightarrow \alpha$, $\kappa a_e^2 \rightarrow \kappa$, $ka_\mu \rightarrow k$, $qa_\mu \rightarrow q$, $r_d/a_\mu \rightarrow r_d$, and $r_D/a_\mu \rightarrow r_D$ are used.

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TABLES

TABLE I. The function $\text{Im}S(t_-)$ for three different values of of the parameter γ and $\sigma = 1.06$.

γ	$\eta(\Omega_0)$	$\text{Im}S(t_-)/\pi$	$w \text{ s}^{-1}$
0.857	21.20	-0.5244	$5.42 \cdot 10^{19}$
1.916	9.48	-1.5130	$3.37 \cdot 10^{44}$
2.710	6.70	-2.2590	$3.03 \cdot 10^{50}$

FIGURES

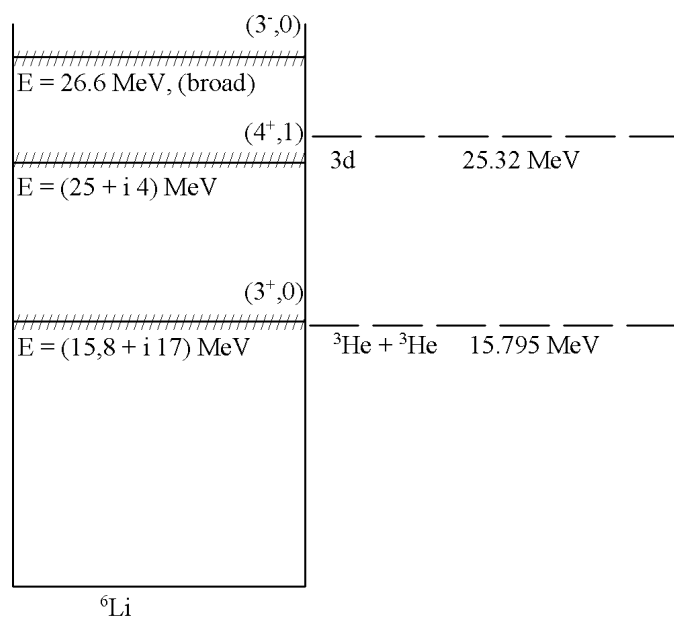


FIG. 1. The ${}^6\text{Li}$ nucleus spectrum.

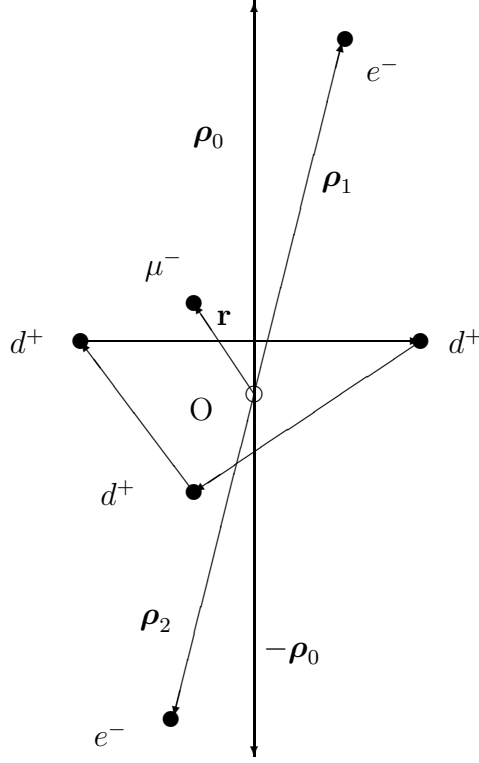


FIG. 2. Jacobi coordinates for all constituent particles of the $D_3\mu$ molecule.

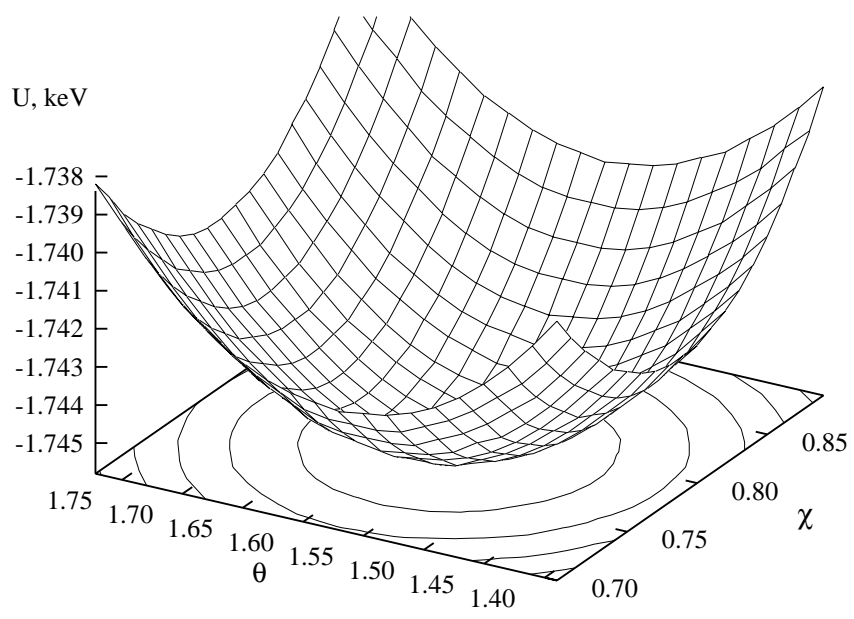


FIG. 3. Two-dimensional cross section of $U(R, \chi, \theta)$ with $R = 4.5 a_\mu$. The surface has a minimum at $\theta = \pi/2$ and $\chi = \pi/4$ which corresponds to the equilateral triangle formed by the 3d nuclei.

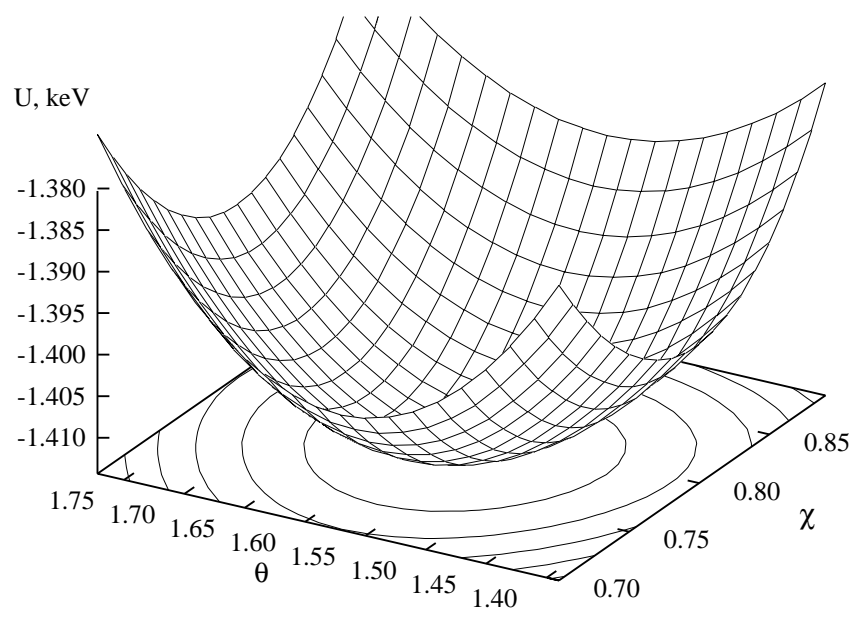


FIG. 4. Same as in Fig. 3 with $R = 2.5 a_\mu$.

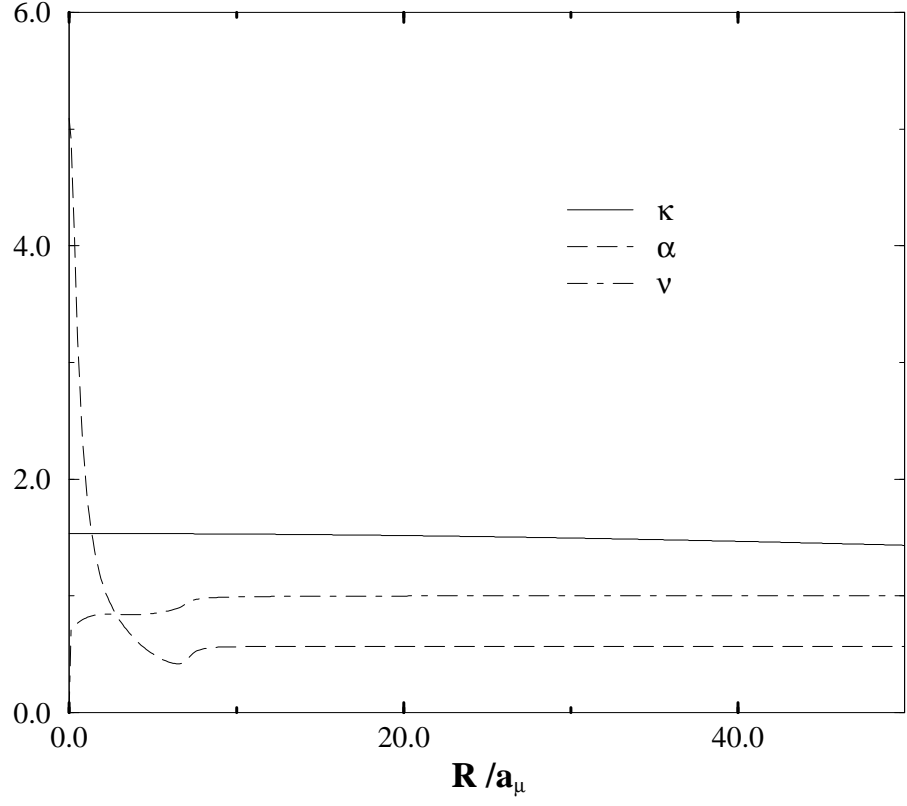


FIG. 5. The dependence of the parameters κ , α , and ν of Eq. (6) on R

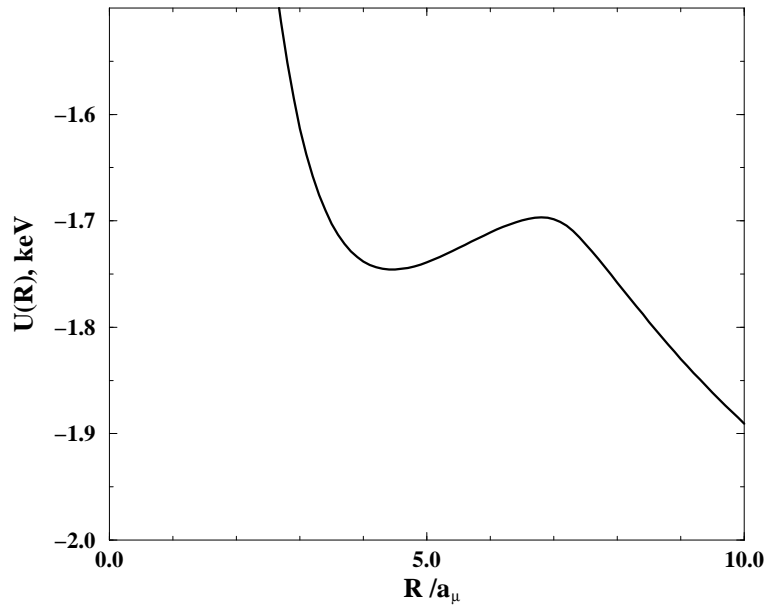
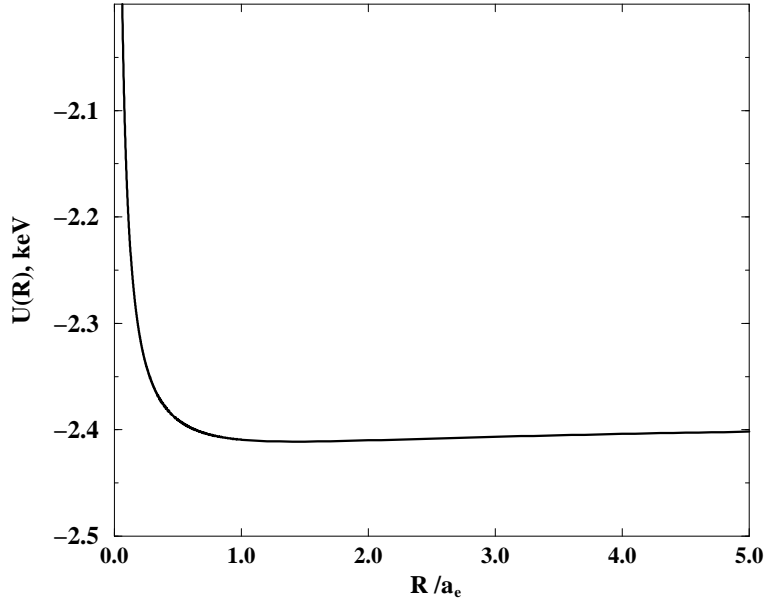


FIG. 6. The $U_0(R) = U(R, \chi_0, \theta_0)$ effective potential. On the upper figure the potential is shown at atomic distances while on the lower at mesonic distances. The a_e and a_μ are the electronic and muonic Bohr radii respectively.